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# SOLUBILITY OF AROMATIC POLLUTANTS IN MIXED SOLVENTS

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## ABSTRACT

The solubility behavior of several aromatic and polynuclear aromatic pollutants was determined in a variety of water/cosolvent mixtures. The data was used to test a log-linear solubility model and develop a relationship for determining the slope of the log-linear solubility curve.

## INTRODUCTION

Predicting the solubility of organic environmental pollutants in mixed solvent systems has become increasingly important in recent years. This is a result of the increased awareness of the importance of solubility in many fate processes.

Pollutants in mixed solvent industrial effluent may remain in solution or may precipitate on contact with water. The ability to predict a system's behavior depends on predicting the mixed solvent as well as the aqueous solubility. Similarly, predicting bio-concentration and toxicity in affected aqueous eco-systems requires an accurate assessment of the exposure concentration (i.e. solubility of the pollutant in the solution phase).

The sorption of organic pollutants from mixed solvent systems to sorbate is "driven" by the activity coefficient in the solution phase (Karickhoff, 1984). Sorption and mixed solvent solubility are inversely related. Rao et al. (1985) have established the inverse relationship between the log of the sorption coefficient and the fraction cosolvent. This is important in modeling the movement of toxic wastes from landfills and in the development of clean up procedures for spills and landfills. The ability to predict solution phase activity, and thus sorption, is vital considering the large number of pollutants involved and the impracticality of collecting the necessary data on each pollutant in each system.

Existing theories address either water solubility or solubility in solvents with a low degree of self-association. These approaches are useful

for extrapolation to mixed solvent systems only when the solvent and cosolvent are very similar.

Yalkowsky et al. (1984) demonstrated a log-linear trend in the solubility vs. fraction cosolvent. Although this relationship holds for a range of solvents and solutes, a degree of deviation was noted in some cases. In this study mixed solvent solubility data were collected for a range of solutes. The data were used to test the generality of the log-linear model and develop a method of predicting the slope of the terminally based log-linear curve.

## EXPERIMENTAL

### Materials

The materials and the abbreviations used in this work are listed below.

| SOLUTES (purity 98% or >) | | |
|---|---|---|
| Name | Abbreviation | Source |
| Anthracene | ANT | 3 |
| Atrazine | ATR | 7 |
| Benzene | BEZ | 8 |
| Biphenyl | BIP | 1 |
| Chrysene | CHR | 1 |
| Diuron | DIU | 7 |
| Naphthalene | NAP | 2 |
| α-Naphthol | NOL | 1 |
| Pyrene | PYR | 1 |
| Phenanthrene | PHN | 1 |
| COSOLVENTS | | |
| Methanol | MOH | 4 |
| Ethanol | EOH | 4 |
| Isopropanol | IPA | 5 |
| Acetone | ACE | 6 |
| Acetonitrile | ACN | 5 |
| Glass-distilled deionized water was used in this project. | | |

1. Aldrich Chemical Co.
2. Alpha Products.
3. Sigma Chemical Co.
4. U.S. Industrial Chemical Co.
5. Fisher Scientific Company.
6. Ashland Chemical Company.
7. Crescent Chemical Co.
8. E.M. Industries Inc.

Solutes were selected to span a range of aromatic hydrocarbons differing in either the number of benzene rings, arrangement or substitution. Anthracene and naphthalene were chosen as reference solutes because of their analytical detectability and because of their well characterized behavior in the solvent systems used in this study.

Binary Solvent Systems

For each binary solvent system studied, a series of mixtures of cosolvent and water are made as follows: 10 ml, 20 ml... 90 ml of cosolvent are mixed with 90 ml, 80 ml, ..., 10 ml of water, respectively. Duplicate aliquots of these mixtures were placed in glass vials with teflon-lined caps. The size of the vials used varied with the system. The solubility of some solutes is so low that the saturated solution had to be injected undiluted (or concentrated) into the HPLC. When this is the case, the saturated solutions were prepared in 10 or 15 ml vials. For solute systems of relatively high solubility 3 ml vials were used.

Liquid solutes were added dropwise to the vials containing the above described cosolvent-water mixtures until a phase separation was obtained. In the case of solid solutes, small increments of solute were added stepwise to the cosolvent-water mixtures contained in the vials until saturation was achieved.

All saturated solutions were equilibrated on a mechanical rotator (14 rpm.) for 18 to 48 hrs. After saturation was achieved, the solutions were centrifuged at 3000 rpm. for 10 minutes in a Beckman model TJ-6 centrifuge. Aliquots of the cosolvent-water phase were analyzed by HPLC-(UV or fluorescence) after appropriate dilution. Dilutions were made with a mixture of acetonitrile-water to prevent phase separation.

Solubility determinations in methanol-water and acetone-water mixtures were made for all solutes. Determinations in ethanol-water, acetonitrile-water, and isopropanol-water mixtures were also made for benzene, naphthalene, and anthracene.

Ternary Solvent Systems

A ternary cosolvent-water system was prepared by adding appropriate amounts of acetonitrile, methanol and water in the manner described above. A complete system of mixtures was prepared, with a change of 10% between the volume fraction of each solvent in the mixture. The ternary solvent systems are water/ACE/MOH, and water/MOH/ACN. The solutes studied in the ternary solvent systems are ANT, BEN, and NAP.

Quinary Solvent Systems

Solubility determinations on quinary solvent systems were performed for benzene, naphthalene, and anthracene. In all cases the solvent system

consisted of mixtures of the following solvents: water, EOH, MOH, IPA, and ACE. The quinary solvent mixtures were prepared by mixing equal proportions of each cosolvent and water. For example, a quinary mixture containing a cosolvent fraction of 0.1 is made with 10% EOH, 10% MOH, 10% IPA, 10% ACE, and 60% water. The volume fraction of the water varied by 20%, from 0 to 100%.

Analytical Methods

The HPLC system consists of two Beckman 110B solvent pumps, a U.V. detector set at 254 nm, and a Beckman analytical optical unit with an 8 ul cell. A Kratos 980 fluorescence detector was used for chrysene. Chromatograms are recorded on a Hewlett-Packard 3390A integrator. The columns used were a 5um Alltech C18 column and a C8 with 250 mm in length and 4.6 mm i.d. The mobile phase used is generally acetonitrile/water (70/30), the flow rate was 1.0 ml/min and the detector range was 0.08. Under these conditions the retention time for the solutes studied ranges from 3 to 15 minutes.

At least 3 standards of known concentration are used with each HPLC run. Each experiment consists of two replicates of eleven samples. Every sample is analyzed at least twice.

Data Analysis

All the raw data were entered into a 'DBASE III' file. The data were then sent to a DEC VAX mainframe and used as input for SAS (statistical analysis system). Terminally based slopes were calculated and linear regressions were then performed using the PROC REG program in the SAS library.

Partitioning Problems

Some solutes, such as benzene and naphthol, form a third phase during equilibration. This third phase is liquid consisting of dissolved solute and cosolvent from the bulk. The preferential partitioning of cosolvent into the third phase changes the volume fraction from the known. In the naphthol/acetone/water system where this occurred the data was not used.

## LOG-LINEAR RELATIONSHIP

Yalkowsky and Roseman (1981) derived an equation expressing the log solubility (moles/liter) of a solute in a mixed solvent system ($S_m$) as the weighted sum of its log solubility in pure cosolvent ($S_c$) and in pure water ($S_w$). Each is weighted by its volume fraction in the mixture ($f_c$ and $f_w$), i.e.

$$\log S_m = f_c \log S_c + (1-f_c) \log S_w \qquad (1)$$

where $f_w$ is replaced by $(1-f_c)$.

Equation (1) assumes that the volume of the solute is much less than the total volume and that the free energy is proportional to the logarithm of the solubility ($\triangle G \propto \log S$). It also assumes that the volume fraction is proportional to the fraction of a molecule in contact with a given solvent.

Assuming a constant $\triangle S_f$, and MP, the solubility equation for each component would be

$$\log S_w = \frac{\triangle S_f\ (MP-25)}{1364} - \log \gamma_w \qquad (2)$$

and

$$\log S_c = \frac{\triangle S_f\ (MP-25)}{1364} - \log \gamma_c \qquad (3)$$

where $\gamma$ is the activity coefficients in the respective solvents. Expressing S in moles/liter introduces little error as long as the solubility is relatively low (Yalkowsky, 1981). The correction factor for differences in the molecularity of the solvents is contained in $\gamma$. Substituting these equations into equation (1) gives

$$\log S_m = \log S_w + f_c(\log \gamma_w - \log \gamma_c) \qquad (4).$$

For a given cosolvent-water system, the difference between the equilibrium activity coefficients in the pure solvents must be constant so that

$$\log \gamma_w - \log \gamma_c = \sigma \qquad (5).$$

Thus equation (4) can be written as

$$\log S_m = \log S_w + f_c\ \sigma \qquad (6).$$

Equation (6) predicts a linear relationship between log $S_m$ and $f_c$ with a slope equal to $\sigma$. This equation assumes the effect of the crystal on the solubility is the same in water, pure cosolvent, or any combination of the two. This does not hold if the solute hydrates in aqueous solutions but not in mixed solvents. The terminally based (ie. end to end) slope is the ratio of the solubility in pure cosolvent ($S_c$) to the water solubility ($S_w$). One or both of these numbers are usually available in the literature or through predictive methods described below.

Similarly, for multiple cosolvent systems, Equation (6) becomes

$$\log (S_m/S_w) = \Sigma\ f_i\ \sigma_i \qquad (7).$$

This predicts that log $S_m$ will vary linearly with $f_i$ if all other concentrations are held constant. This relationship was observed by Rubino (1984) for several drugs in mixed solvents and by Yalkowsky et al. for a range of pollutants in cosolvent-water systems (EPA report #CR811852-01-0).

Predicting σ

The terminally based slope, σ, of the log S vs. fraction cosolvent curve may be represented by Equation (5). Similarly, the octanol-water partition coefficient of the solute (P) is

$$\log P = \log (\gamma_w / \gamma_o) \qquad (8).$$

Where $\gamma_w$ and $\gamma_o$ are the activity coefficients in the water and octanol respectively.

Since the log activity coefficient in a cosolvent is proportional to that in octanol (for hydrophobic interactions), σ can be written as

$$\sigma = a \log P + b \qquad (9).$$

Where a and b are the slope and intercept of the σ vs. log P curve.

Equation (9) predicts that within a solvent system the terminally based slope of the log-linear solubility curve is proportional to the solutes' octanol-water partition coefficient.

Mixed Solvent Solubility From σ and Log P

Yalkowsky and Valvani (1980) developed a semi-empirical method of predicting the water solubility of nonelectrolytes based on melting point and partition coefficient at 25°C.

$$\log S_w = -\log P - 0.01(MP-25) + 0.8 \qquad (10)$$

where P is the partition coefficient, $S_w$ is the solubility (moles/liter) and MP is the melting point of the compound in degrees centigrade. The partition coefficient can be estimated by the group contribution values of Nys and Rekker.

Expressed in mg/ml Equation (10) becomes

$$\log S_w = -\log P - 0.01(MP-25) + 0.8 + \log MW \qquad (11)$$

where MW is the molecular weight of the solute.

Substituting the semi-empirical relationships for σ and log $S_w$ into Equation (6) results in a general equation for mixed solvent solubility.

$$\log S_m = (a \log P + b) f_c - \log P - 0.01(MP-25) + 0.8 + \log MW \qquad (12)$$

Equations of this form would allow prediction of mixed solvent solubility given a, b, MP and log P values (MP is assumed to be 25° for liquids).

## RESULTS

### Binary Cosolvent-Water Systems

Solute solubility in the various binary cosolvent-water mixtures show a reasonable log-linear relationship according to Equation (6). The solubility data is plotted for six solutes in the methanol/water system (Figure 1) and for naphthalene in six solvent systems (Figure 2). Since the endpoints of each curve are fixed, the only reasonable measure of agreement with the model is the deviation from the log-linear line. The average absolute deviation and average factor of deviation are presented for each 10% increase in cosolvent for the figures shown. Table I shows that the maximum average error did not exceed a factor of 3 for any of the twelve systems. Table II lists the terminally based slopes for all solutes in the systems studied.

Of the systems studied methanol/water usually shows the least deviation from the model for a given solute. Figure 2 shows naphthalene in all the binary systems including the systems of acetone/water and isopropanol/water which show the most deviation from the model. The average deviations presented are typical of the remaining systems studied.

### Higher Order Cosolvent-Water System

Solubility in higher order cosolvent mixture can also be treated as the weighted sum of the log solubilities in the individual volume fractions of the solvents. For example, the solubility (mg/ml) of naphthalene in the ternary cosolvent system of ACN, MOH, and water can be described by the following equation.

$$\log S = 3.86(ACN) + 3.39(MOH) - 1.59 \qquad (13)$$

where ACN and MOH are the volume fractions of acetonitrile and methanol respectively in the ternary solvent mixtures, and the $\sigma$ values are from Table I.

Solubility in the quinary solvent mixture consisting of equal amounts of acetonitrile, methanol, ethanol, and isopropanol with varying amounts of water is treated as above. The equation for predicting the solubility of anthracene follows directly from the results in Table I.

$$\log S = 4.61(ACN) + 4.29(EOH) + 4.13(IPA) + 4.21(MOH) - 4.26 \qquad (14)$$

where the intercept is taken to be the average of the water solubilities for the respective binary systems.

Equations such as (14) can be reduced to a simpler form if the volume fraction of each cosolvent is the same. In this case, the results would be a

FIGURE 1: LOG Sm vs FRACTION METHANOL

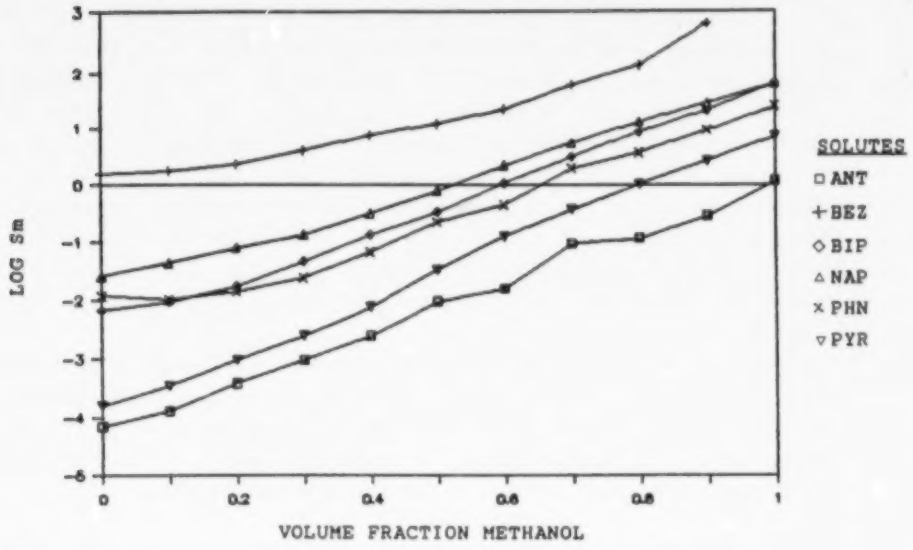



FIGURE 2: LOG Sm vs FRACTION COSOLVENT

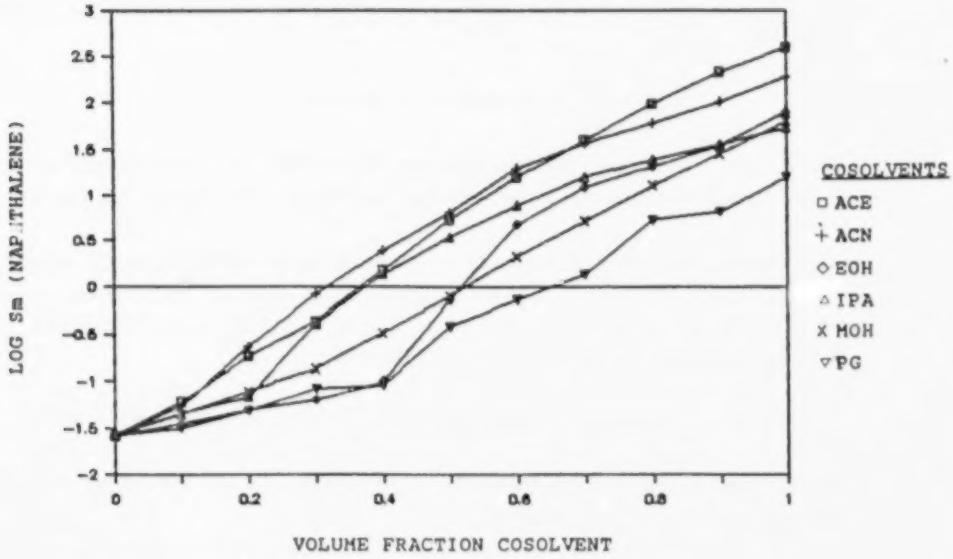


TABLE I

| FRACTION COSOLVENT | AVERAGE ABSOLUTE DEVIATION | | AVERAGE FACTOR OF ERROR | |
|---|---|---|---|---|
| | HEO SYSTEMS | NAP SYSTEMS | HEO SYSTEMS | NAP SYSTEMS |
| 0 | 0 | 0 | 0.0 | 0.0 |
| 0.1 | 0.25 | 0.13 | 1.8 | 1.3 |
| 0.2 | 0.33 | 0.21 | 2.1 | 1.6 |
| 0.3 | 0.37 | 0.31 | 2.3 | 2.0 |
| 0.4 | 0.32 | 0.46 | 2.1 | 2.9 |
| 0.5 | 0.26 | 0.37 | 1.8 | 2.3 |
| 0.6 | 0.24 | 0.31 | 1.7 | 2.0 |
| 0.7 | 0.15 | 0.28 | 1.4 | 1.9 |
| 0.8 | 0.13 | 0.17 | 1.3 | 1.5 |
| 0.9 | 0.1 | 0.09 | 1.3 | 1.2 |
| 1 | 0 | 0 | 0.0 | 0.0 |

TABLE II

TERMINALLY BASED SLOPES IN BINARY SYSTEMS
σ values

| | | COSOLVENTS | | | | |
|---|---|---|---|---|---|---|
| | | MOH | ACE | EOH | ACN | IPA |
| | BEN | 2.06 | 1.94 | 2.05 | 1.73 | 1.95 |
| S | NAP | 3.39 | 4.17 | 3.48 | 3.86 | 3.32 |
| O | ANT | 4.21 | 5.22 | 4.29 | 4.61 | 4.13 |
| L | BIP | 3.97 | 4.80 | 4.09 | ..... | |
| U | PYR | 4.30 | 5.36 | ..... | | |
| T | CRY | 4.96 | 6.11 | ..... | | |
| E | NOL | 2.78 | ..... | | | |
| S | ATR | 2.40 | 2.63 | ..... | | |
| | DIU | 2.27 | 2.51 | ..... | | |
| | PHN | 3.31 | 4.24 | ..... | | |

linear sum of the coefficients from such equations. For naphthalene and anthracene respectively the equations are

$$\log S = 14.15(f_c) - 1.59 \quad (15)$$

$$\log S = 17.24(f_c) - 4.26 \quad (16).$$

A linear regression of the solubility measurements in the quinary cosolvent-water systems against fraction cosolvent yields the following equations.

$$\log S = 14.9(f_c) - 1.67 \quad (17)$$
$$n = 6 \quad s = 0.138 \quad r = 0.996$$

$$\log S = 19.1(f_c) - 4.16 \quad (18)$$
$$n = 6 \quad s = 0.085 \quad r = 0.995$$

The favorable comparison of these two sets of equations show that the solubility of naphthalene and anthracene in these multicomponent systems can be treated as the weighted sum of the log solubility in the individual volume fractions of the solvents.

Prediction of $\sigma$

The terminally based slopes of all the solutes in a given solvent system were analyzed with the 'PROC REG' linear regression program contained in SAS. Binary cosolvent systems from Yalkowsky et al. (1986) were also included. The resulting values for a and b, as well as, the adjusted r-squared values are presented in Table III. The high degree of correlation over several orders of magnitude of log P make these equations useful estimators of $\sigma$. The low $r^2$ for the EG systems is due to the low slope of the curve. The $\sigma$ values for chrysene and phenanthrene in acetone and methanol were predicted before they were measured. The experimental and predicted values for these systems are within a few percent of each other.

Substituting the proper a and b values from Table III into Equation (9) gives the equation for $\sigma$ in the acetone-water systems

$$\sigma = 0.997 \log P + 0.484 \quad (19).$$
$$\text{adj. } r^2 = .927$$

Figure 3 is the plot of $\sigma$ vs log P for the acetone/water solvent system.

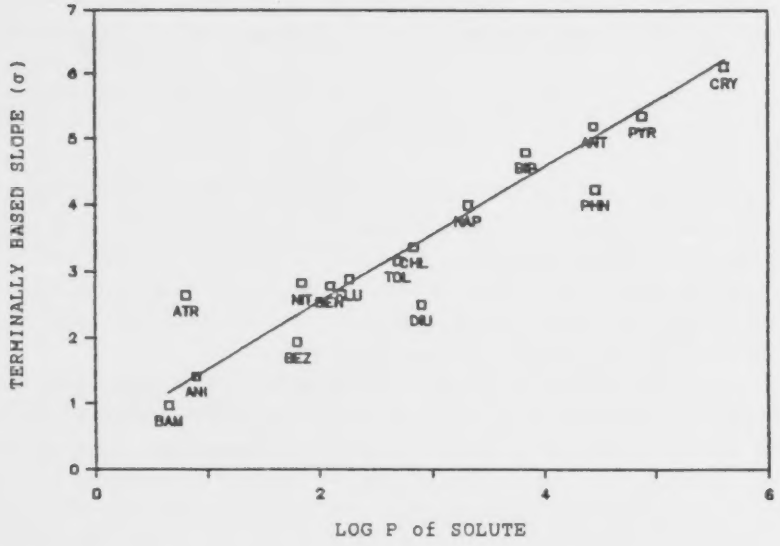
Atrazine was not included in the regressions because of its anomalous solubility behavior between 0 and 10% cosolvent. This will be discussed below.

TABLE III

SUMMARY OF REGRESSIONS PARAMETERS FOR TERMINAL SLOPE (σ) VS. LOG P IN EACH BINARY SOLVENT SYSTEM:

| COSOLVENT/WATER SYSTEM | R SQUARED (adjusted) | n | (a) | (b) |
|---|---|---|---|---|
| ACETONE | 0.93 | 14 | 1.00 | 0.48 |
| ACETONITRILE | 0.90 | 8 | 1.03 | 0.35 |
| DIMETHYLACETAMIDE | 0.95 | 7 | 0.86 | 0.89 |
| DIMETHYLFORMAMIDE | 0.94 | 7 | 0.87 | 0.87 |
| DIMETHLYSULFOXIDE | 0.95 | 7 | 0.89 | 0.87 |
| ETHYLENE GLYCOL | 0.75 | 7 | 0.36 | 1.04 |
| ETHANOL | 0.94 | 11 | 0.85 | 0.81 |
| ISOPROPANOL | 0.85 | 9 | 0.89 | 0.63 |
| METHANOL | 0.84 | 16 | 0.68 | 1.07 |
| PROPYLENE GLYCOL | 0.96 | 8 | 0.62 | 0.77 |

FIGURE 3: SIGMA vs LOG P, ACETONE/WATER



When experimental values for solute solubility in the pure cosolvent were unavailable due to the complete miscibility of the solute, the density of the solute was substituted (eg; benzene).

Mixed Solvent Solubility Prediction

Substituting the a, b, MP, and log P values into Equation (12) for the systems of chrysene and atrazine in acetone/water, produces the predictions listed in Table IV. Neither of these solutes was included in the regression for the a and b values used here (a=1.02, b=0.5).

The model does a good job of predicting the solubility of chrysene between the end points with maximum deviation at the end points. The variation can be reduced by a factor of two to ten by using Yalkowsky's equation specific for polynuclear aromatics. Even without the correction, an order of magnitude prediction is available in minutes.

Atrazine exhibits anomalous solubility behavior, and may violate one of the assumptions of the model. It is possible that atrazine forms a hydrate in water but not in the presence of cosolvent. The model assumes that the crystal has the same impact on solubility irrespective of the solvent. Its water solubility could certainly be better estimated using an equation designed for its class of compound. Yet, if the predicted water solubility is ignored the rest of the predictions are within an average factor of 5.4 from the observed values. Considering the fact that the acetone/water system usually shows significant deviation, this represents a good test of the model.

## CONCLUSIONS

The log-linear model does a reasonable job of describing the solubility behavior of the solutes in the solvent systems studied. The maximum error is less than an order of magnitude, usually substantially less. Extending the log-linear model to higher order systems is a simple matter of adding the products of the binary solvent systems $\sigma$'s and volume fraction, to the water solubility for the solute of interest.

The relationship between log P and $\sigma$ described makes it possible to determine mixed solvent solubility *a priori* in the systems characterized. The mixed solvent solubility in the systems studied are immediately available using the fragment constants of Nys and Rekker to predict log P, Yalkowsky's equation for water solubility, and the equation for $\sigma$ from Table III. Using the specific water solubility equation should allow predictions within a factor of three.

The utility of the model lies in its simplicity. Only three components are needed to estimate the solubility of a solute in a mixed aqueous solvent of any composition: the a and b values for the binary solvent system, and the

TABLE IV

CHRYSENE AND ATRAZINE IN ACETONE/WATER SYSTEMS

| FRACTION COSOLVENT | LOG S observed | LOG S predicted | DEVIATION (obs-pred) |
|---|---|---|---|
| CHRYSENE | | | |
| 0.00 | -5.68 | -4.75 | -0.93 |
| 0.20 | -3.53 | -3.51 | -0.02 |
| 0.40 | -2.68 | -2.26 | 0.42 |
| 0.60 | -1.19 | -1.02 | -0.17 |
| 0.80 | -0.30 | 0.23 | -0.53 |
| 1.00 | 0.43 | 1.47 | -1.04 |
| ATRAZINE | | | |
| 0.00 | -1.14 | 0.85 | -1.99 |
| 0.10 | 0.10 | 0.98 | -0.88 |
| 0.20 | 0.40 | 1.11 | -0.71 |
| 0.30 | 0.54 | 1.25 | -0.71 |
| 0.40 | 0.69 | 1.38 | -0.69 |
| 0.50 | 0.78 | 1.51 | -0.73 |
| 0.60 | 0.77 | 1.64 | -0.87 |
| 0.70 | 1.03 | 1.78 | -0.75 |
| 0.80 | 1.25 | 1.91 | -0.66 |
| 0.90 | 1.42 | 2.04 | -0.62 |
| 1.00 | 1.49 | 2.18 | -0.69 |

solute's MP and log P.

A complete tabulation of the data is available from U.S. Environmental Protection Agency, R.S. Kerr Environmental Research Laboratory, Ada, Oklahoma.

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